Pumping spin-chain materials and the emergence of generalized Gibbs ensembles

Zala Lenarčič, Florian Lange, Achim Rosch
University of Cologne

- theory of weakly driven quantum system
- "Novel (quantum) state" out of equilibrium
- spin and heat pump
- Floquet states in open systems

Lenarčič, Lange, A.R., arXiv:1706.05700
Lange, Lenarčič, A.R., Nature Comm. 8, 15767 (2017)

QM2 Quantum Matter & Materials

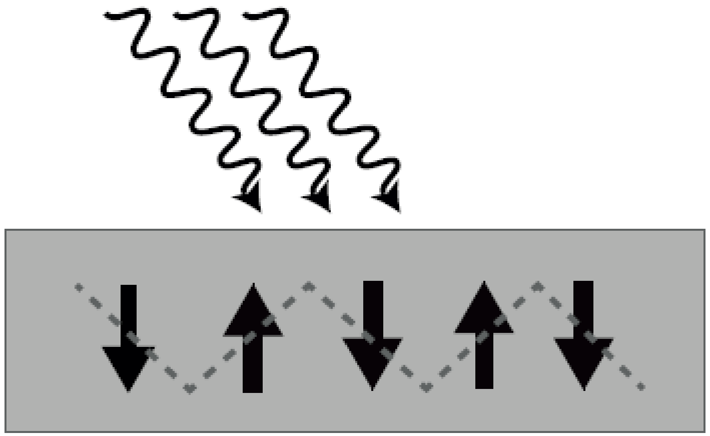
CRC183 ENTANGLED STATES OF MATTER

CRC1238 Control and Dynamics of Quantum Materials

weakly driven many-particle systems:
strong, qualitative effects (beyond linear response)?

e.g. laser on a solid, weakly shake cold atom system

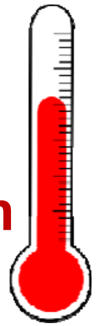
- (quantum-) phase transitions
- pumping into resonances
- **approximate conservation laws**



weakly driven systems: refrigerator

picture of fridge removed
for copyright reasons

inside fridge:



out-of-equilibrium but
approximate equilibrium
with temperature ***T***

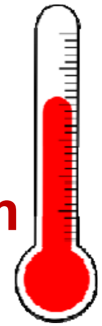
essential:
energy inside fridge approximately conserved due to insulation

weakly driven systems: refrigerator

picture of fridge

inside fridge:

out-of-equilibrium but
approximate equilibrium
with temperature T_{fridge}

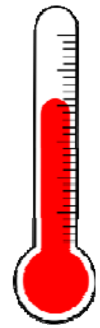


essential:
energy inside fridge approximately conserved due to insulation

weakly driven systems: refrigerator

picture of fridge

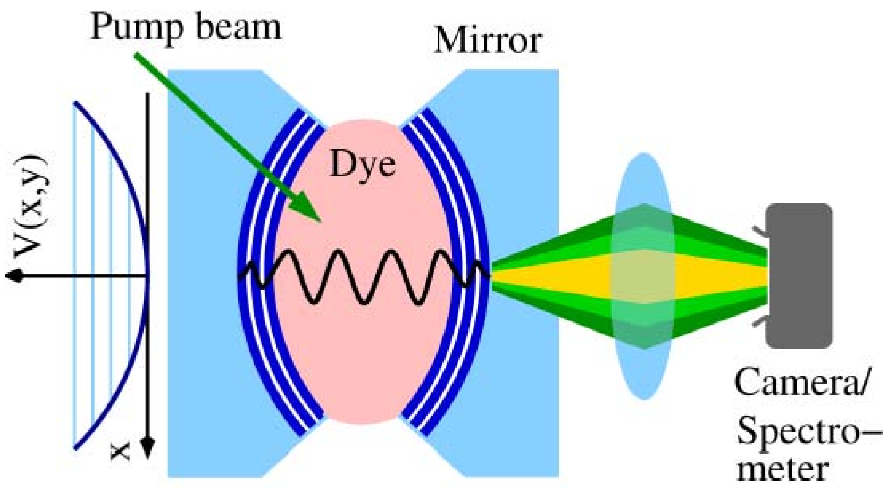
calculate T_{fridge}



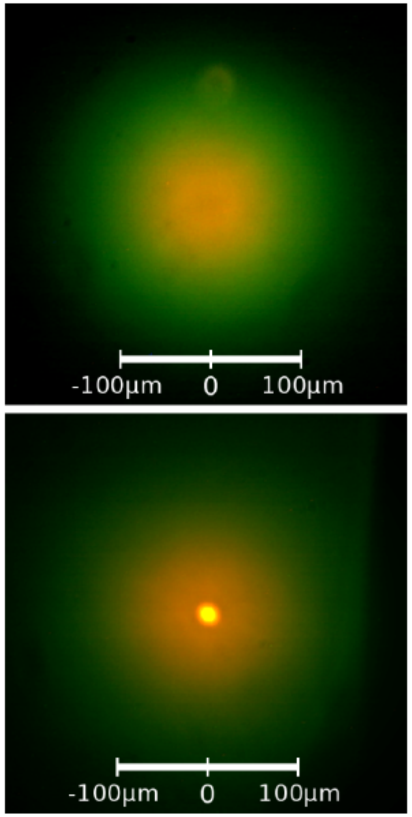
rate equation:

incoming energy current
=
outgoing energy current

Weakly driven systems: Bose-Einstein condensation of photons



Weitz group Bonn, Nature 2010
quantum greenhouse

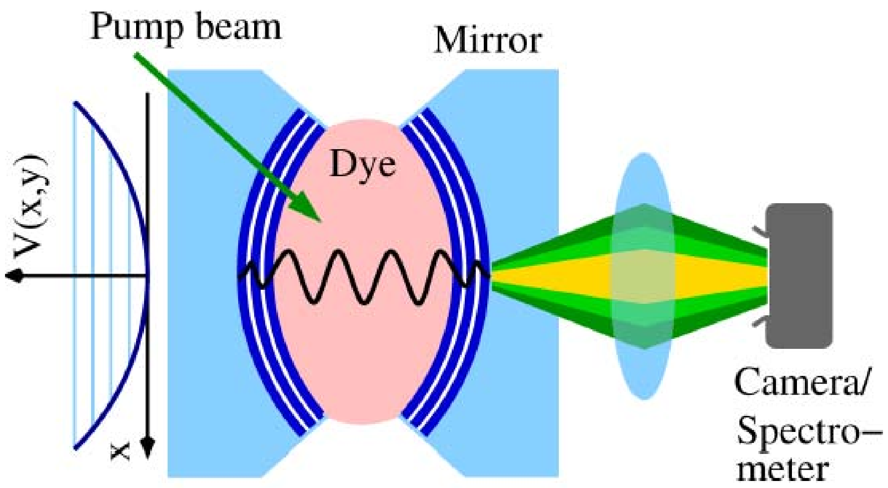


slightly increased pump intensity

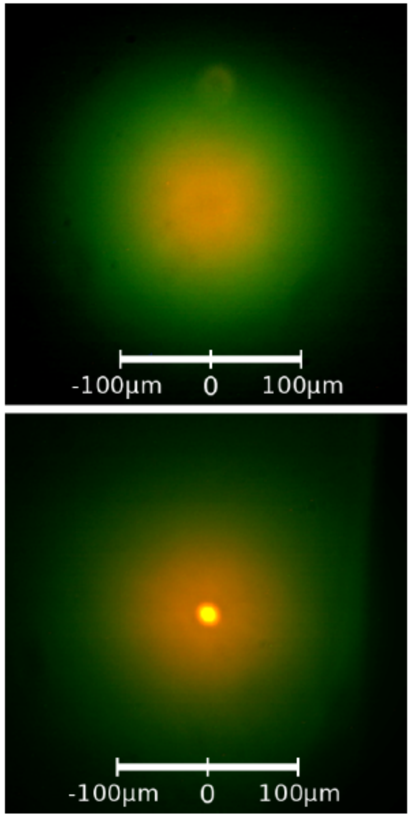
BEC of photons at **room temperature**

photon number **approximately conserved**
photon losses through mirrors/ non-radiative decay of dye molecules

Weakly driven systems: Bose-Einstein condensation of photons



Weitz group Bonn, Nature 2010
quantum greenhouse



slightly increased pump intensity

BEC of photons at **room temperature**

thermal equilibration of photons
by frequent absorption/emission from thermalized dye molecules

➡ accurate description by Gibbs ensemble with chemical potential μ for photons

$$n_B(\epsilon_n) = \frac{1}{\exp[(\epsilon_n - \mu)/T] - 1}$$

eco-fridge principle: pump approximately conserved charges

goals

- derive **systematic perturbation theory** for weakly driven quantum many-particle system
- activation of exotic approximate conservation laws, study **approximately integrable systems**
- useful? New types of heat- or spin **pumps**

definition: weakly driven many-particle quantum system

time evolution of density matrix: $\partial_t \rho = \mathcal{L}\rho$ $\qquad t \to \infty$

with **Liouville super-operator** $\mathcal{L} = \mathcal{L}_0 + \epsilon\, \Delta\mathcal{L}, \qquad 0 < \epsilon \ll 1$

leading order: Hamiltonian time evolution with conservation laws C_i

$$\mathcal{L}_0 \rho = -i[H_0, \rho] \qquad \mathcal{L}_0 C_i = 0$$

C_i = energy, particle number, conserved charges of integrable systems….

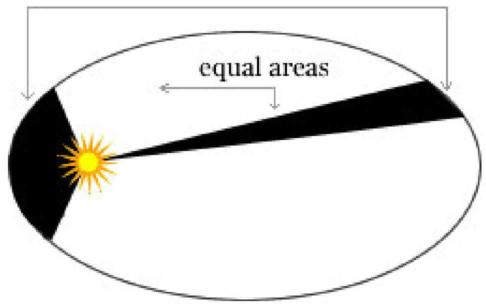
$$\Delta\mathcal{L} = \begin{cases} \text{periodic perturbation} \quad H_1(t) = e^{-i\omega_0 t} H_1 + e^{i\omega_0 t} H_1^\dagger \\ \text{phonons, integrabiliy breaking terms, …} \\ \text{coupling to non-thermal bath described by Lindblad operators} \end{cases}$$

Integrable systems

number of conservation laws = number of degrees of freedom

for classical, few-particle systems:

- example: Kepler problem, harmonic oscillator, …
- regular orbits even under weak perturbation (KAM theorem)



many-particle quantum systems

- examples: 1d Hubbard model, 1d Heisenberg model,
  1d bosons (Lieb-Liniger), also: many-body localization
- O(N) quasi-local conservation laws (N = # of sites)
- solvable by Bethe ansatz techniques (not used here)

Integrable systems

special case: **integrable systems** in 1d

here: xxz chain

$$H_0 = \sum_j J(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + \Delta S_j^z S_{j+1}^z$$

special: exactly solvable due to **infinite** (O(N)) number of local and quasi-local conserved charges C_i

$$\begin{aligned} C_1 &= \sum S_i^z \\ C_2 &= H_0 \\ C_3 &= \textbf{heat current} \\ &= J^2 \sum \vec{S}_i \cdot \left(\vec{S}_{i+1} \times \vec{S}_{i+2}\right) \quad \text{for } \Delta = 1 \\ C_4 &= \ldots \end{aligned}$$

spin current: not exactly conserved but finite overlap with quasi-local conservation law (Prosen, 2011)

Reminder: thermal Equilibrium

$$\rho \sim e^{-(H-\mu N)/k_B T}$$

one free parameter
(temperature, chemical potential)
per conservation law

Equilibration of integrable systems: more conservation laws

replace notion of Gibbs ensemble by

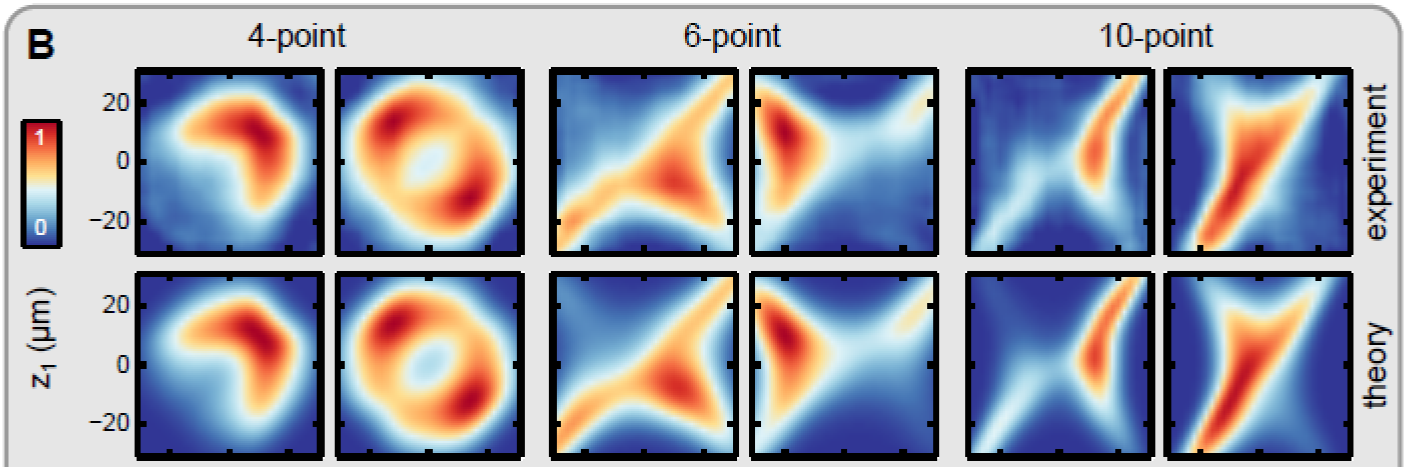
generalized Gibbs ensemble (GGE)

$$\rho \sim e^{-\sum_i \lambda_i C_i}$$

Jaynes (1957), Rigol *et al*. (2007)

belief: **describes long-time limit after quantum quench exactly**

experiments with ultracold atoms (Lieb-Liniger model):
Schmiedmayer group, Science 2015



Exactly integrable systems

generalized Gibbs ensemble (GGE)

$$\rho \sim e^{-\sum_i \lambda_i C_i}$$

but: in solids **perturbations**
(phonons, interchain couplings, disorder,…)
break integrability weakly

coupling to a **thermal** bath

$$\rho_{\mathrm{th}} \sim e^{-\lambda_1 C_1} = e^{-\beta H_0}$$

this talk:
coupling **non-thermally**
reactivates GGE for weak integrability breaking

$$\rho_{\mathrm{GGE}} \sim e^{-\sum_i \lambda_i C_i}$$

picture of fridge removed

generalized Gibbs ensemble

$$\rho \sim e^{-H_{\mathrm{fridge}}/T_{\mathrm{fridge}} - H_{\mathrm{room}}/T_{\mathrm{room}}}$$

good approximation despite the fact that H_{fridge} only approximately conserved. GGE established due to weak driving!

search for **stationary states** for $\epsilon \ll 1$

stationary state (if it exists):
$\Delta\mathcal{L} = const.$

$$\rho(t \to \infty)$$

for periodically driven system:
$\Delta\mathcal{L}(t) = \Delta\mathcal{L}(t+T),$
$\omega_0 = 2\pi/T$
use **Floquet density matrix**

$$\rho(t \to \infty) = \sum_n e^{-i\omega_0 n t}\rho_n$$

typically: $\rho_n \propto \epsilon^n$

in the following: $\rho = (\ldots, \rho_{-1}, \rho_0, \rho_1, \ldots)$ $\rho_n^\dagger = \rho_{-n}$

weakly driven system: $O(\epsilon^0)$

$$\partial_t \rho = \mathcal{L}\rho \qquad \mathcal{L} = \mathcal{L}_0 + \epsilon\,\Delta\mathcal{L}$$

$$\lim_{\epsilon\to 0} \rho(t \gg 1/\epsilon) \quad \textbf{?}$$

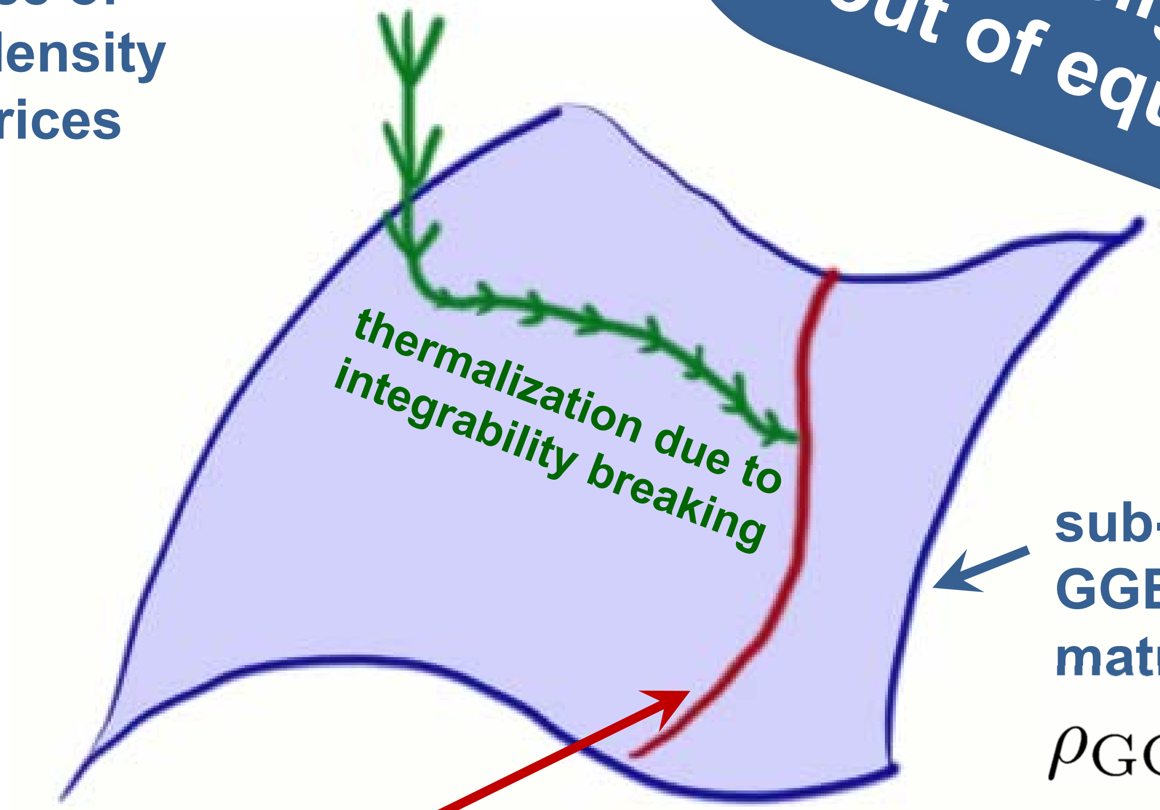
$$\mathcal{L}_0\rho = -i[H_0, \rho] \approx 0$$

$$\lim_{\epsilon\to 0} \rho(t \gtrsim 1/\epsilon) = \rho_{\mathrm{GGE}}(t) \sim e^{-\sum_i \lambda_i^0(t) C_i}$$

relaxation in approximately integrable systems (no driving terms):

What happens when system is slightly perturbed out of equilibrium ?

space of all density matrices



sub-space of GGE density matrices

$$\rho_{\mathrm{GGE}} \sim e^{-\sum_i \lambda_i C_i}$$

$$\rho_{\mathrm{th}} \sim e^{-\lambda_1 C_1} = e^{-\beta H_0}$$

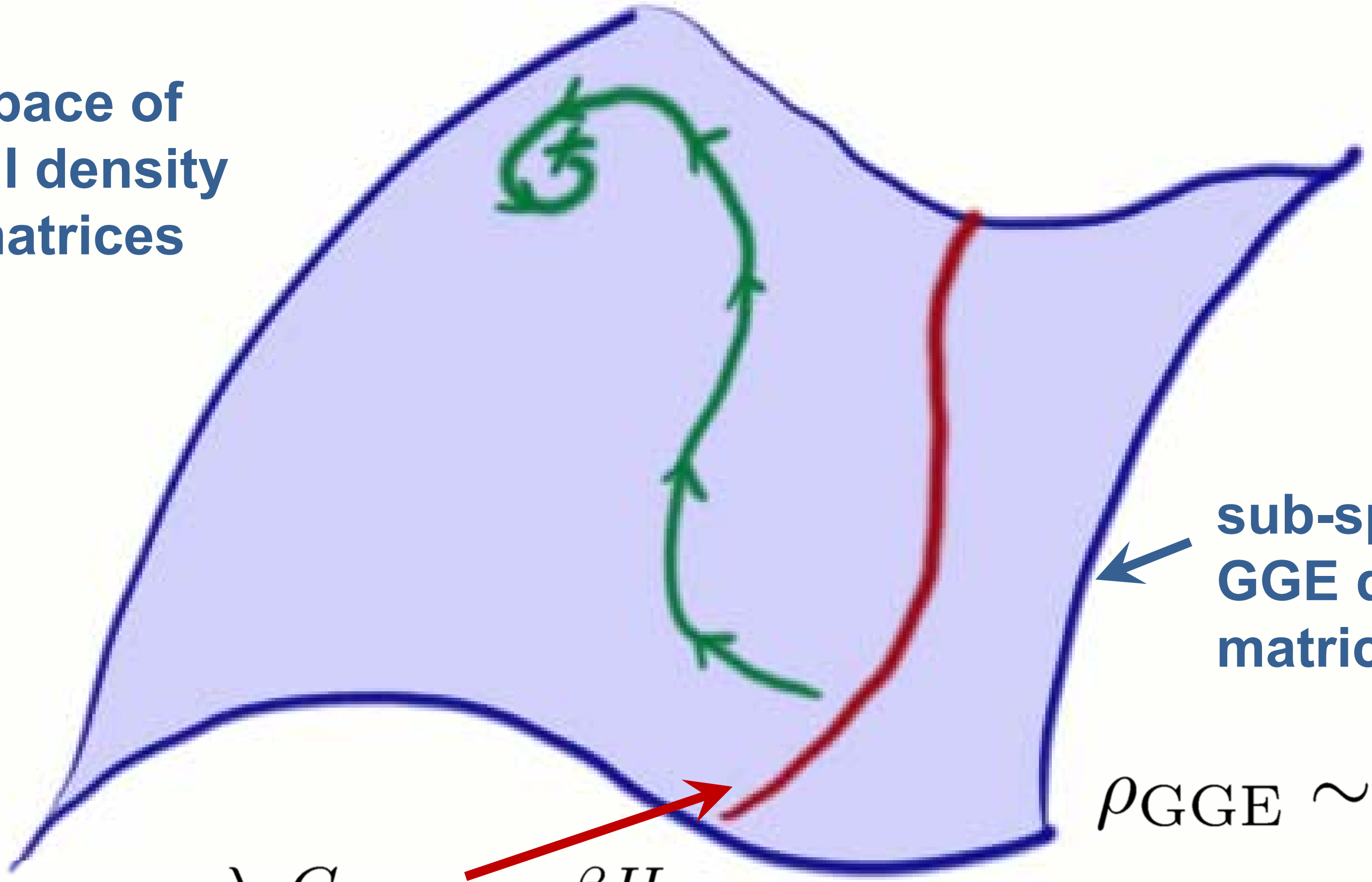
eco-fridge principle: pump approximately conserved charges

weakly driven system:
losses compensated by pumping

weakly driven system: $O(\epsilon^0)$

$$\mathcal{L} = \mathcal{L}_0 + \epsilon\, \Delta\mathcal{L}$$

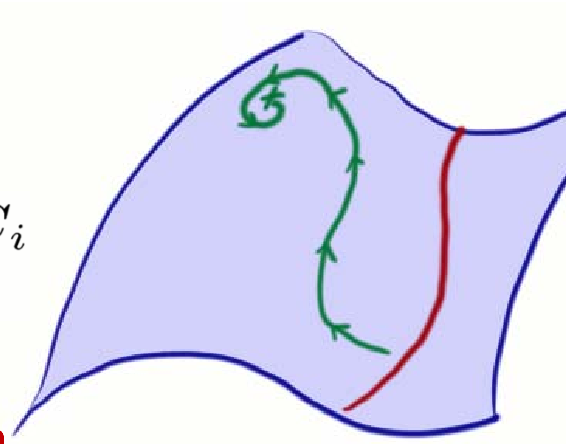
$$\lim_{\epsilon \to 0} \rho(t \gtrsim 1/\epsilon) = \rho_{\mathrm{GGE}}(t) \sim e^{-\sum_i \lambda_i^0(t) C_i}$$



weakly driven system: $O(\epsilon^0)$

$$\mathcal{L} = \mathcal{L}_0 + \epsilon\, \Delta\mathcal{L}$$

$$\lim_{\epsilon\to 0} \rho(t \gtrsim 1/\epsilon) = \rho_{\mathrm{GGE}}(t) \sim e^{-\sum_i \lambda_i^0(t) C_i}$$



determine time evolution of λ_i^0 from **rate equation for approximately conserved charges**:

$$\langle \partial_t C_i \rangle = \mathrm{tr}[C_i \partial_t \rho] \approx \epsilon\, \mathrm{tr}[C_i\, \Delta\mathcal{L}(\rho_{\mathrm{GGE}})]$$

often leading order vanishes, then use (Golden rule):

$$\langle \partial_t C_i \rangle \approx \epsilon^2\, \mathrm{tr}\left[C_i\, \Delta\mathcal{L}\mathcal{L}_0^{-1}\, \Delta\mathcal{L}\, \rho_{\mathrm{GGE}})\right]$$

evaluated by exact diagonalization of H_0

Numerical check:
Heisenberg chain perturbed by Lindblad dynamics

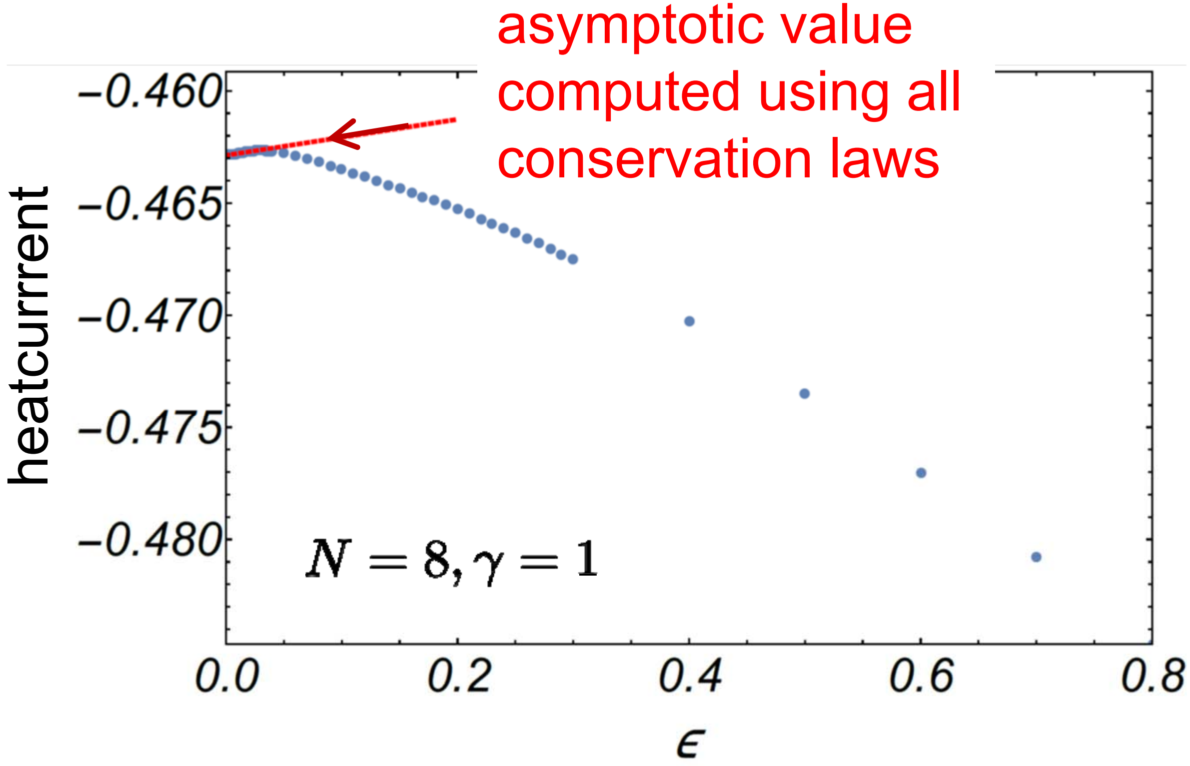
$$\partial_t \rho = \mathcal{L}\rho \qquad \mathcal{L} = \mathcal{L}_0 + \epsilon \Delta\mathcal{L}$$

$$\mathcal{L}_0 \rho = -i[H_0, \rho] \qquad H_0 = J \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1}$$

$$\Delta\mathcal{L} = \gamma \Delta\mathcal{L}_1 + (1-\gamma)\Delta\mathcal{L}_2 \qquad \Delta\mathcal{L}_i\, \rho = \sum_j L_i^{j\dagger} \rho L_i^j - \frac{1}{2}\{L_i^{j\dagger} L_i^j, \rho\}$$

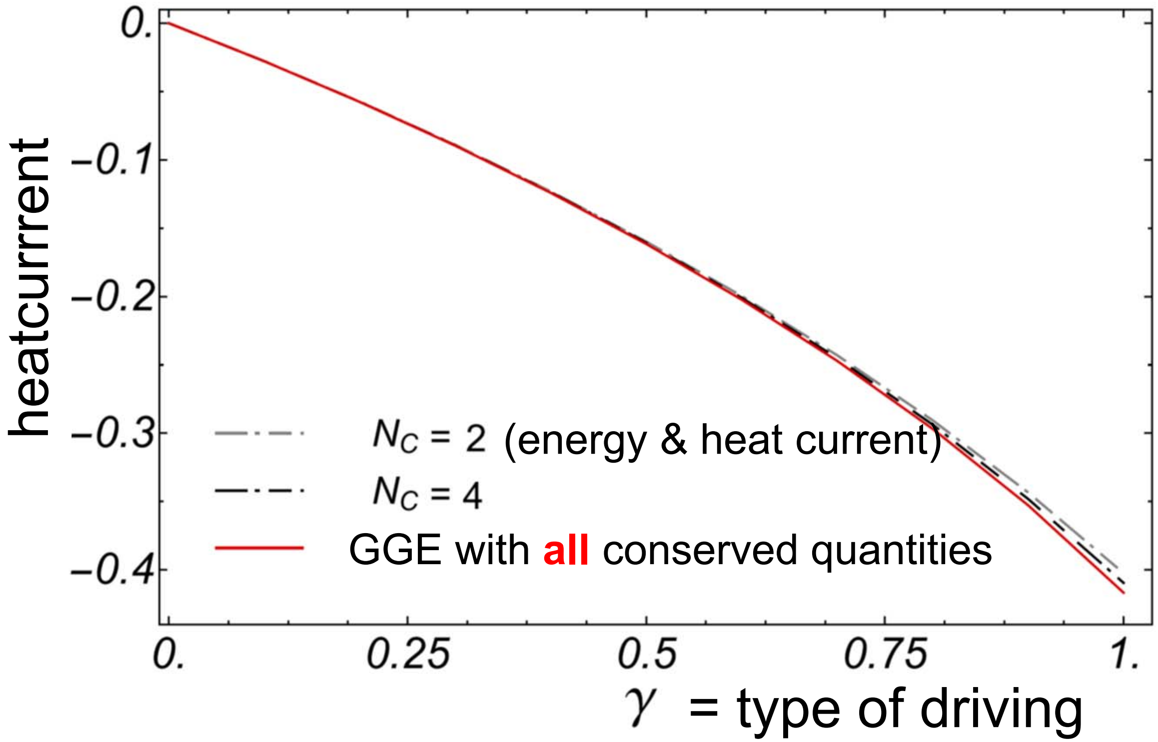
$$L_1^j = \sigma_j^+ \sigma_{j+1}^- + \sigma_{j+1}^- \sigma_{j+2}^+ \qquad L_2^j = S_i^z$$

giant heat current even for infinitesimally weak perturbation



Numerical check:
Heisenberg chain perturbed by Lindblad dynamics

Do we need all conseration laws or do a few conservation laws already capture GGE?

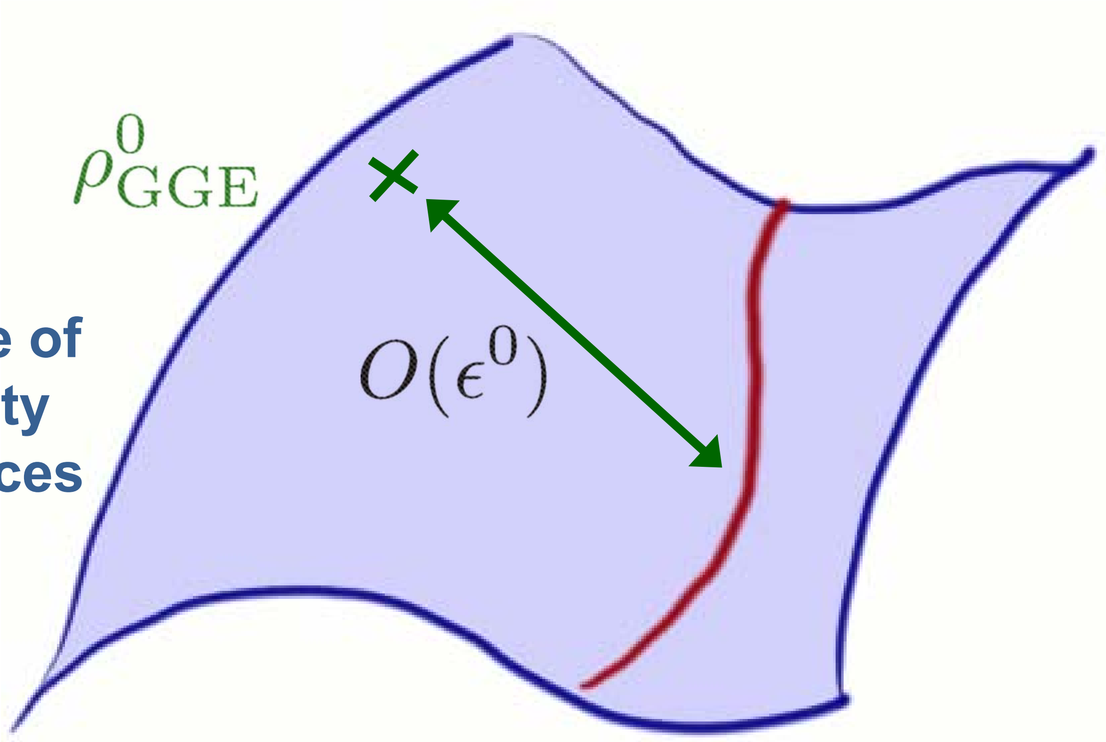


this example:
truncated GGE with just 2-4 conservation laws accurately describes weak driving limit

Perturbation theory for stationary states: $O(\epsilon^0)$

$$\mathcal{L} = \mathcal{L}_0 + \epsilon\,\Delta\mathcal{L}$$
$$\lim_{\epsilon\to 0} \rho(t=\infty) = \rho_{\mathrm{GGE}} \sim e^{-\sum_i \lambda_i^0 C_i}$$

space of density matrices



next order ?

problem:
zero modes of $\mathcal{L}_0$

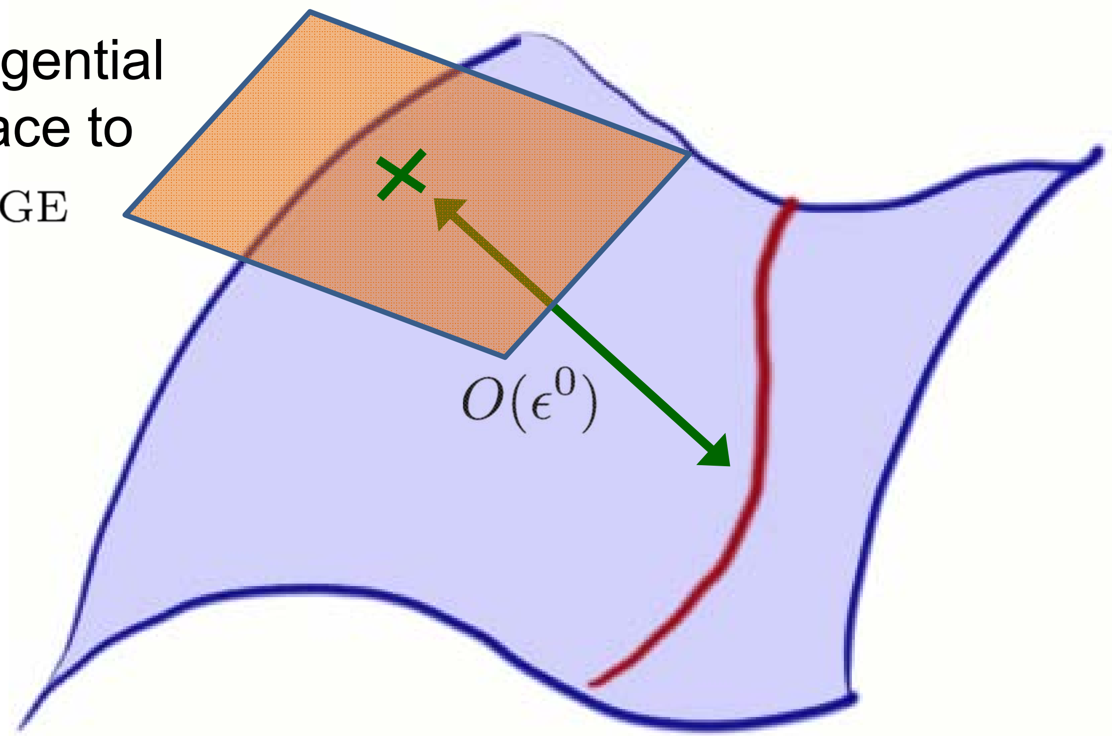
Perturbation theory for stationary states

needed:
super-operator **P** projecting on space tangential to GGE ensembles
(similiar Mori-Zwanzig memory matrix formalism)

$$\mathbf{P}[X] = \sum_i \frac{\partial \rho_{GGE}}{\partial \lambda_i} (\chi^{-1})_{ij} \,\mathrm{tr}[C_j X]$$

$$\chi_{ij} = \frac{\partial \langle C_i \rangle_{\mathrm{GGE}}}{\partial \lambda_j^0}$$

tangential space to ρ_{GGE}

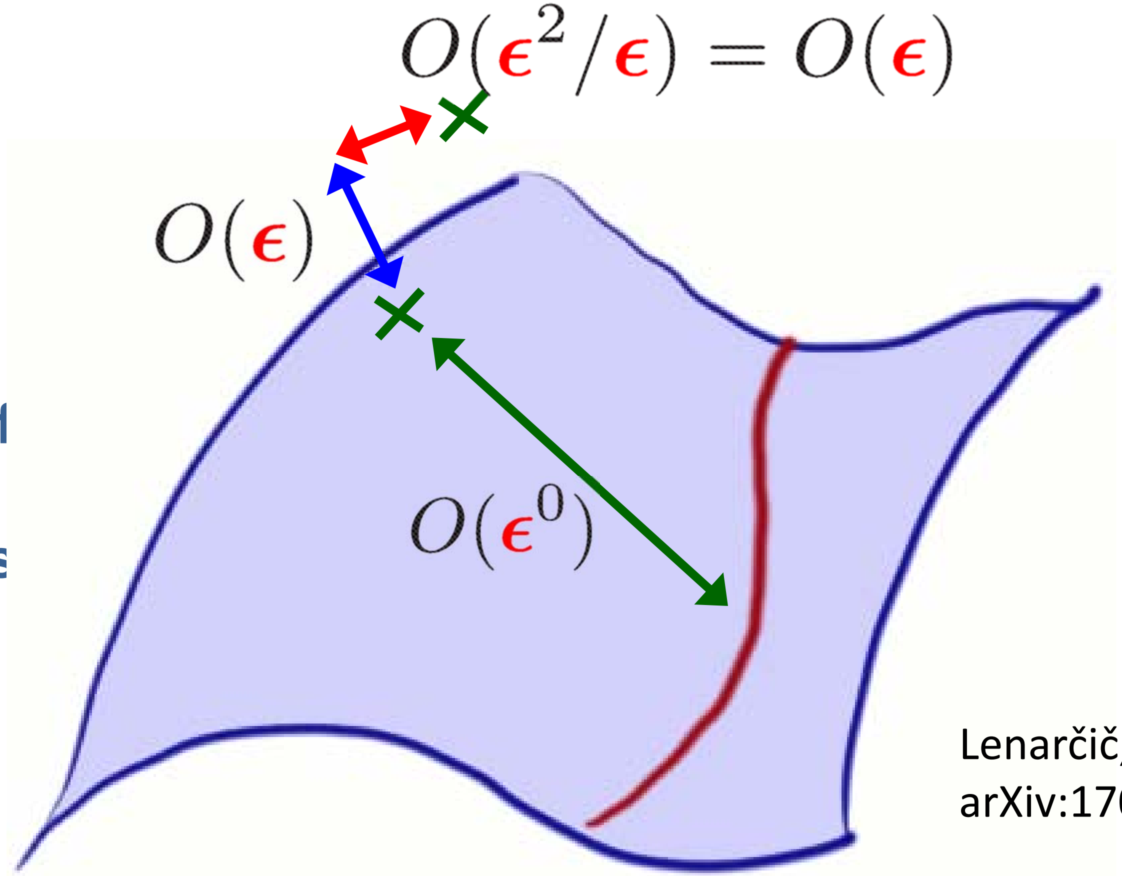


- projector: $\mathbf{P}^2 = \mathbf{P}$
- projector in perpend. direction $\mathbf{Q} = 1 - \mathbf{P}$
  $\mathbf{QP} = \mathbf{PQ} = 0$
- $\mathcal{L}_0 \mathbf{P} = \mathbf{P} \mathcal{L}_0 = 0$

Perturbation theory for stationary states

$$\delta\rho = -\epsilon\,\underbrace{(\mathcal{L}_0)^{-1}\,\Delta\mathcal{L}\,\rho^0_{\mathrm{GGE}}}_{\perp \text{ to } \rho^0_{\mathrm{GGE}}} + \underbrace{\frac{\epsilon^2}{\epsilon}\,(\mathbf{P}\,\Delta\mathcal{L}\,\mathbf{P})^{-1}\,\mathbf{P}\Delta\mathcal{L}\,(\mathcal{L}_0)^{-1}\,\Delta\mathcal{L}\,\rho^0_{\mathrm{GGE}}}_{\parallel \text{ to } \rho^0_{\mathrm{GGE}}}$$

space of density matrices



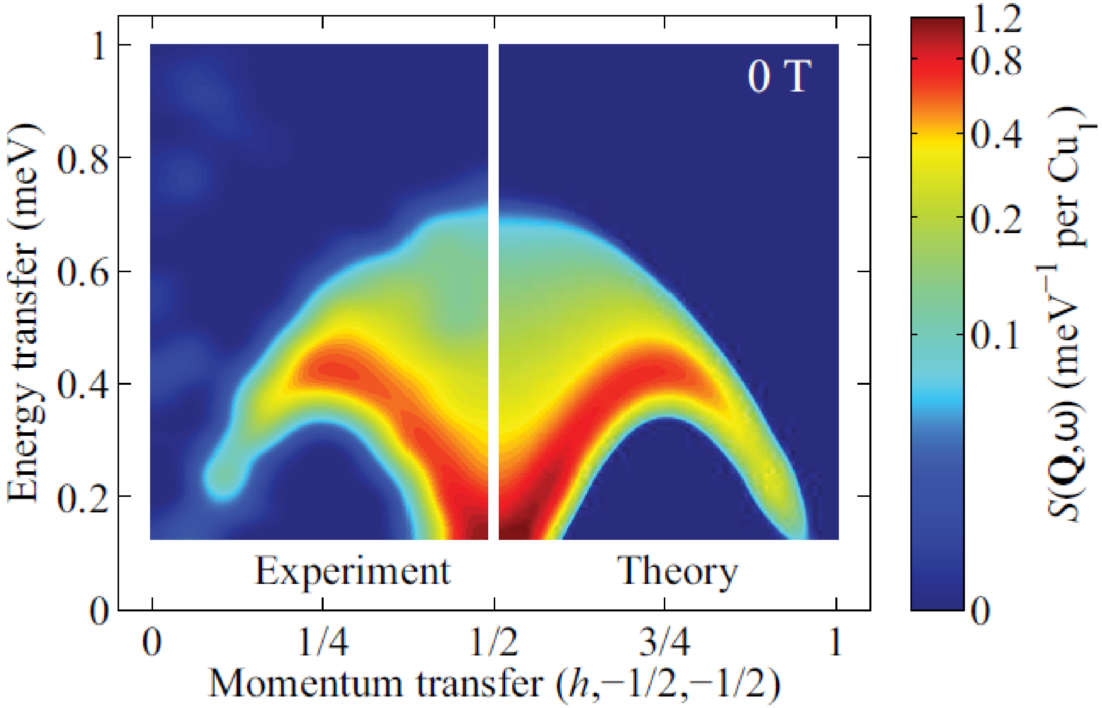
Lenarčič, Lange, A.R., arXiv:1706.05700

now: something useful

use: **heat current** conserved in xxz chain

goal: build **heat pump** using spin-chain materials many accurate experimental realizations of xxz-Heisenberg models measured in thermodynamics, neutron scattering, …

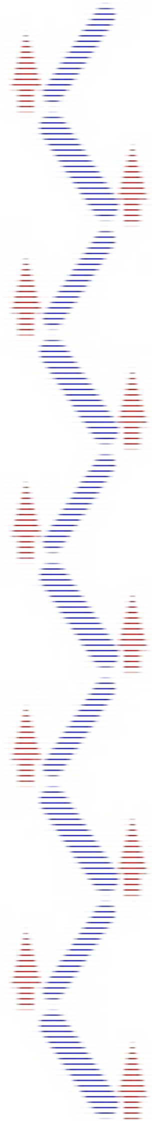
e.g. cupper sulphate pentahydrate, $CuSO_4 \cdot 5D_2O$
Ronnow & Caux groups, Nature Physics 2013



simplified model $\mathcal{L} = \mathcal{L}_0 + {\color{red}\epsilon} \left(\mathcal{L}_{\mathrm{pump}} + \mathcal{L}_{\mathrm{bath}} \right)$

$$H_0 = \sum_j J(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + \Delta S_j^z S_{j+1}^z - B \sum_j S_j^z$$

$$H_{\mathrm{pump}} = E_0 \sum_j (-1)^j \cos(\omega_0 t)\, \mathbf{S}_j \mathbf{S}_{j+1} + B_0 \sum_i (-1)^j \sin(\omega_0 t) S_j^z$$



e.g., R. Shindou (2005):
in adiabatic limit, T=0: quantized spin pump (Thouless)

here opposite limit: large T, large ω_0, small amplitudes

simplified model $\mathcal{L} = \mathcal{L}_0 + \epsilon\left(\mathcal{L}_{\text{pump}} + \mathcal{L}_{\text{bath}}\right)$

$$H_0 = \sum_j J(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + \Delta S_j^z S_{j+1}^z - B \sum_j S_j^z$$

$$H_{\text{pump}} = E_0 \sum_j (-1)^j \cos(\omega_0 t)\, \mathbf{S}_j \mathbf{S}_{j+1} + B_0 \sum_i (-1)^j \sin(\omega_0 t) S_j^z$$

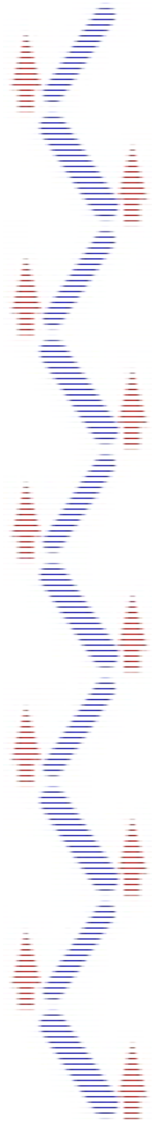
to avoid unlimited heating:
couple to bath of, e.g., phonon

$$H_{\text{bath}} = \sum_j \epsilon_0 a_j^\dagger a_j + \lambda \sum_j \mathbf{S}_j \mathbf{S}_{j+1}(a_j^\dagger + a_j) + H_{\text{res}}$$

assume: phonons always thermalized with $T = T_{\text{ph}}$
by coupling to further reservoirs

Can this realistically be realized in solids? YES !

wave-length of light >> lattice constant



Create time-dependet staggered B-fields and Heisenberg coupling:

trick: use Heisenberg-chain materials with low symmetries

Oshikawa, Affleck 1997

staggered B-fields experimentally **observed**, e.g., in

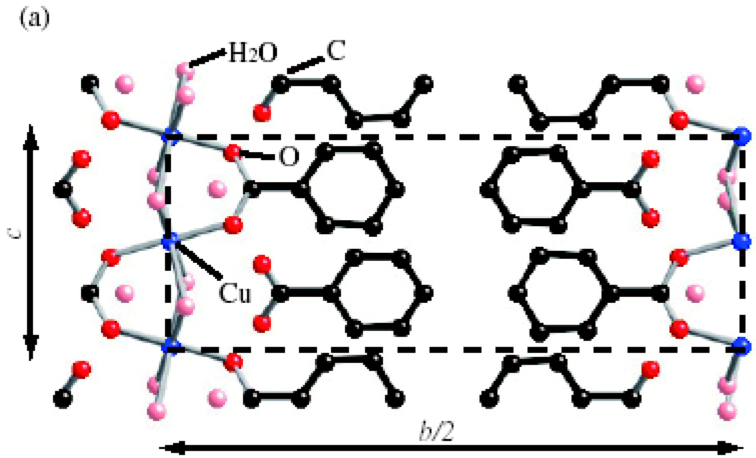
$Cu(C_6H_5CO_2)_2 \cdot 3H_2O$ (Cu benzoate, blue flame in fireworks)

Nojiri et al. (2006), Aeppli et al. (1997)

Yb_4As_3 Iwasa et al. (2002)

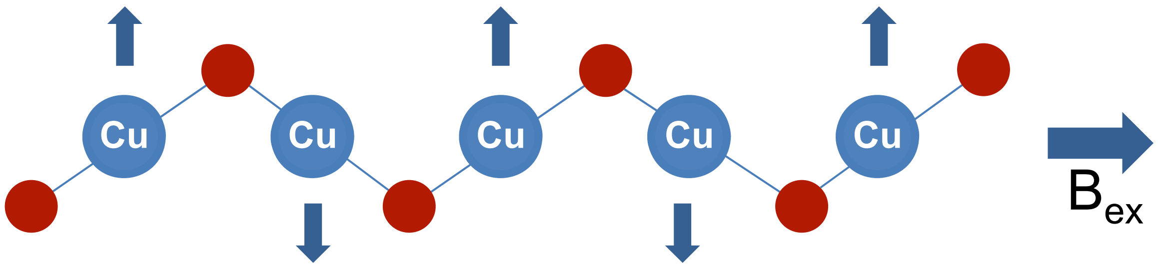
$BaCo_2V_2O_8$ Chen et al. (2013)

$CuCl_2 \cdot 2((CD_3)_2 SO)$ Broholm et al (2007)

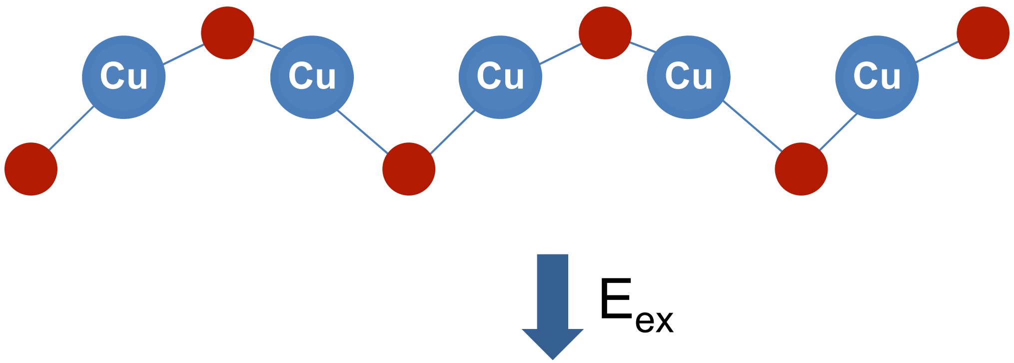


Nojiri et al. (2006)

Cu benzoate



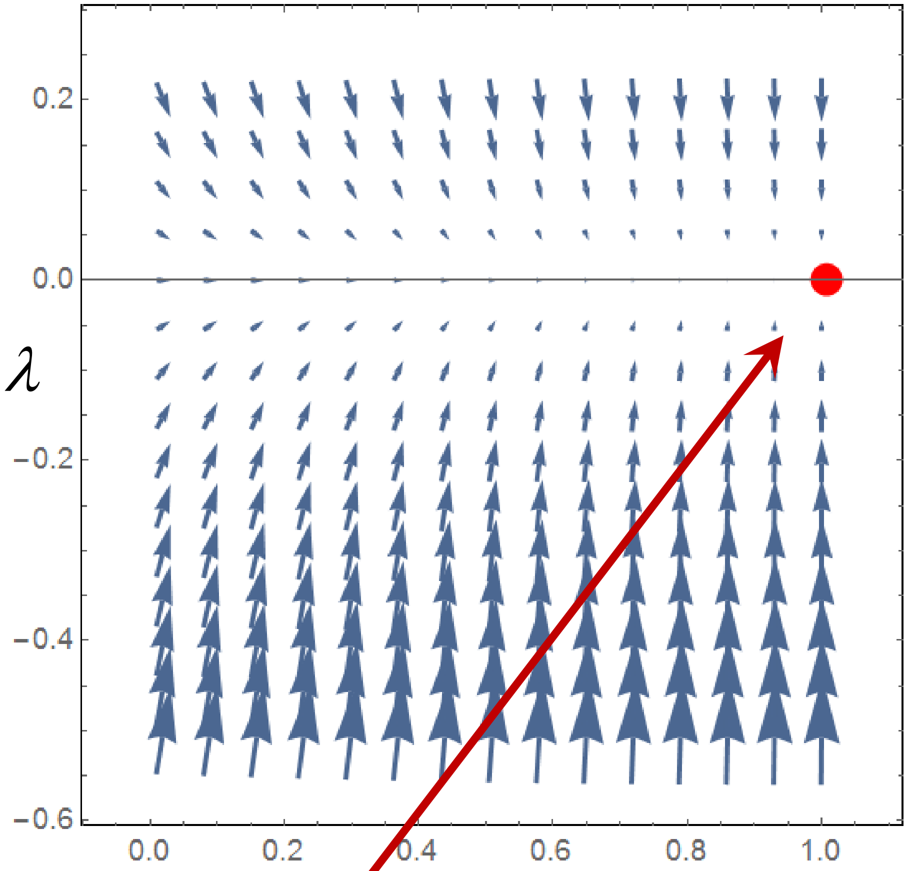
staggered
B-field



staggered
exchange

$$\rho_{\mathrm{GGE}} \sim e^{-\beta H - \lambda J_H} \qquad \partial_t(\beta,\lambda) = \vec{F}(\beta,\lambda)$$

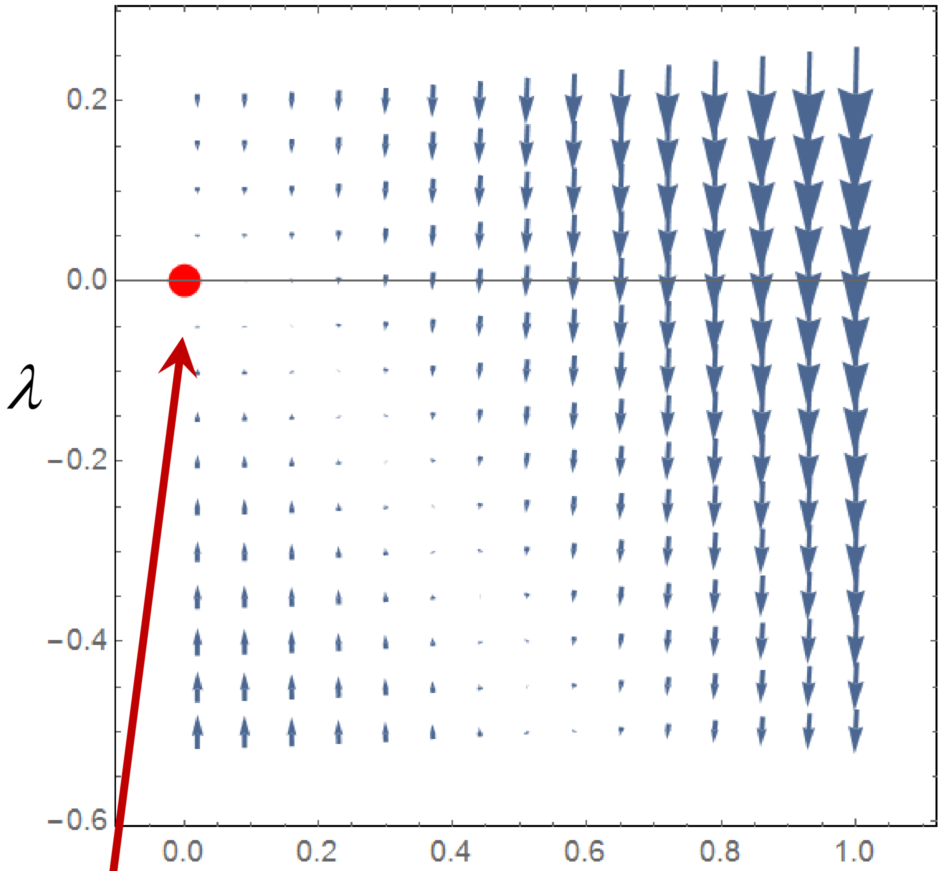
only phonons, no driving



β = 1/T

flow towards phonon T
no heat current λ=0

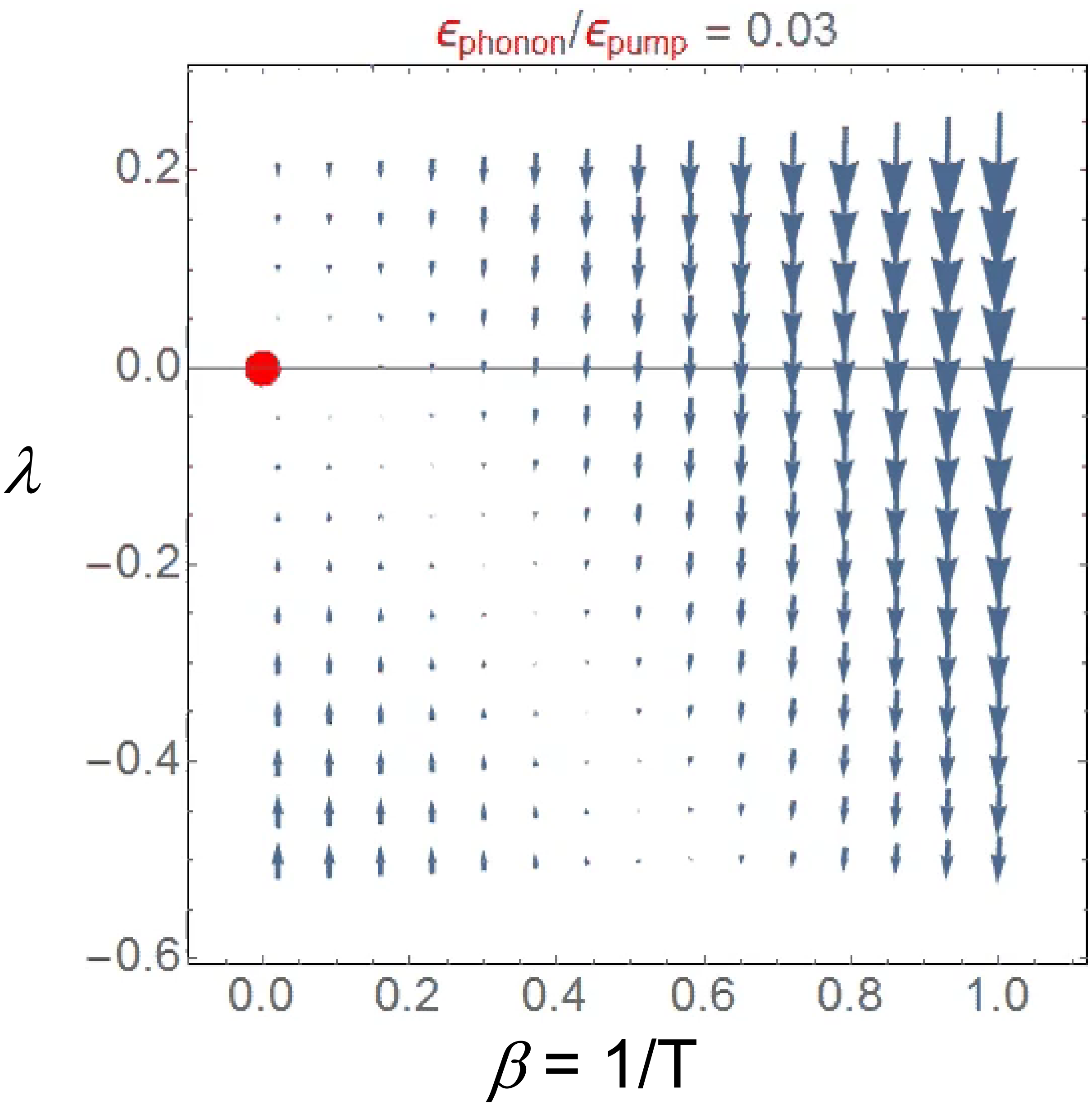
only periodic driving, no phonons



β = 1/T

T=∞ fixed point
no heat current λ=0

steady state depends on ratio of coupling constants



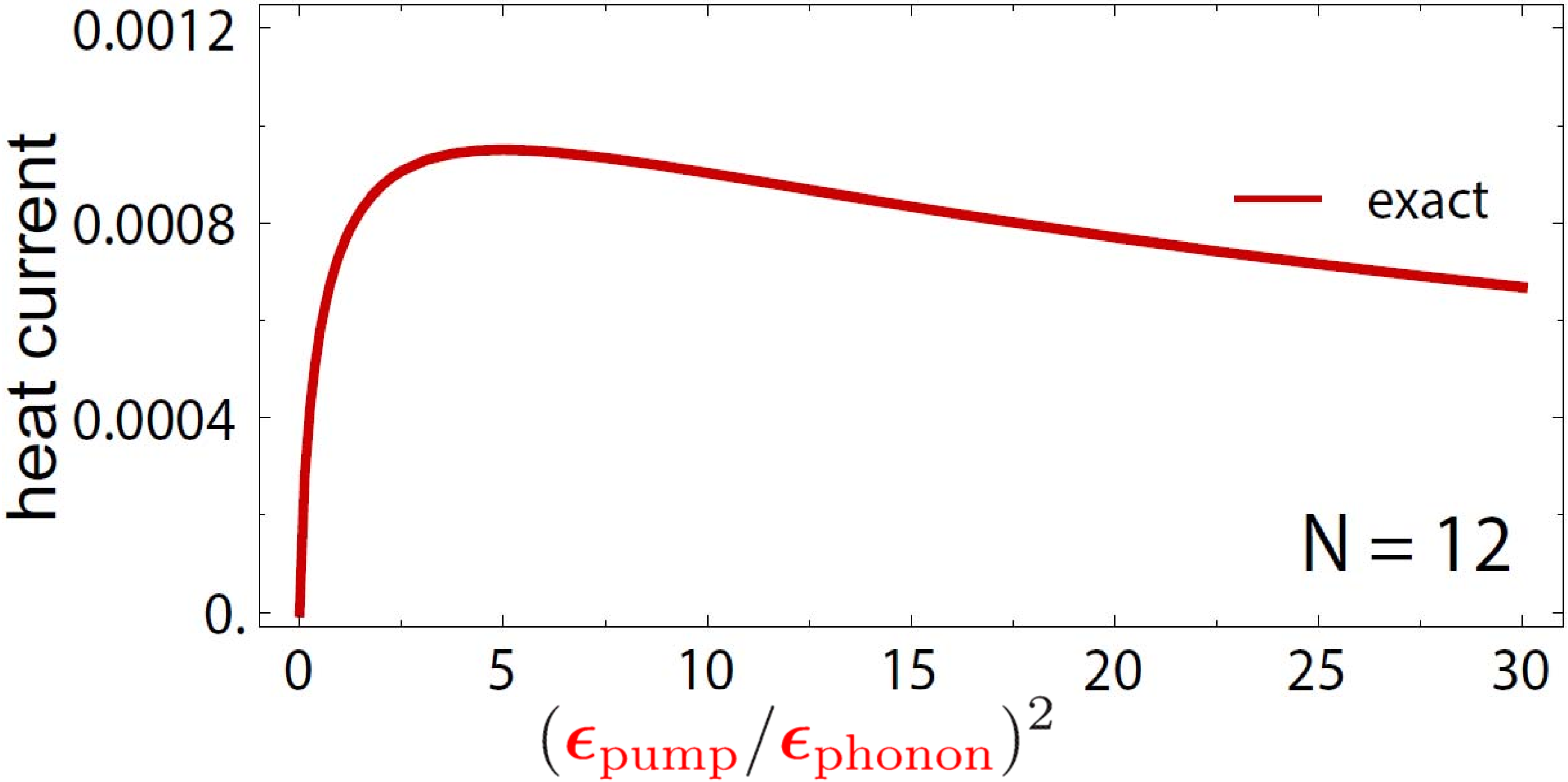
parameters:

$T_{\rm ph} = J, \Delta = J/2,$

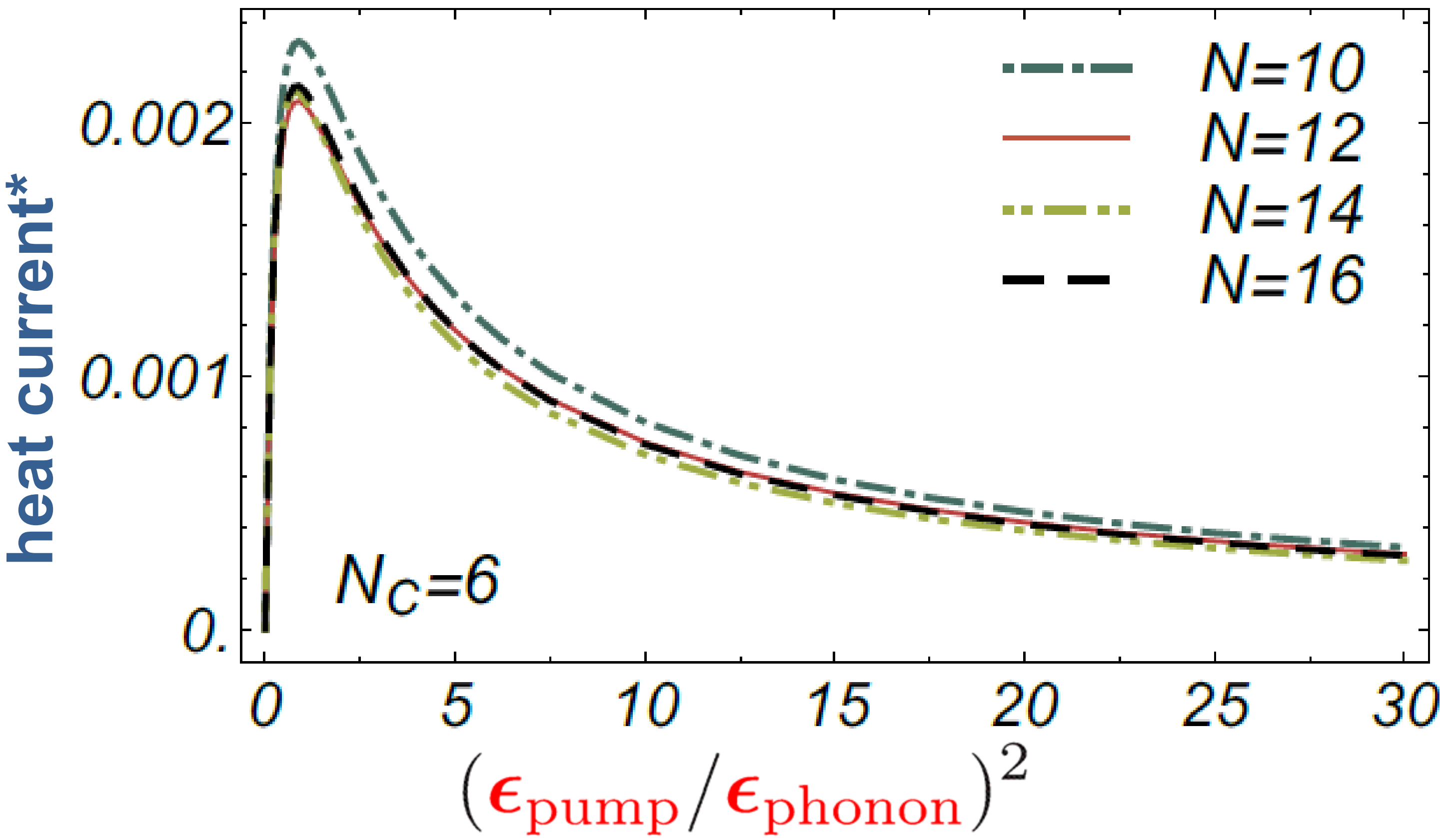
$\omega_0 = 1.5J, B = 0.8\,J,$

$\epsilon_0 = J, E_0/B_0 = 1$

$$\rho_{\rm GGE} \sim e^{-\beta H - \lambda J_H}$$

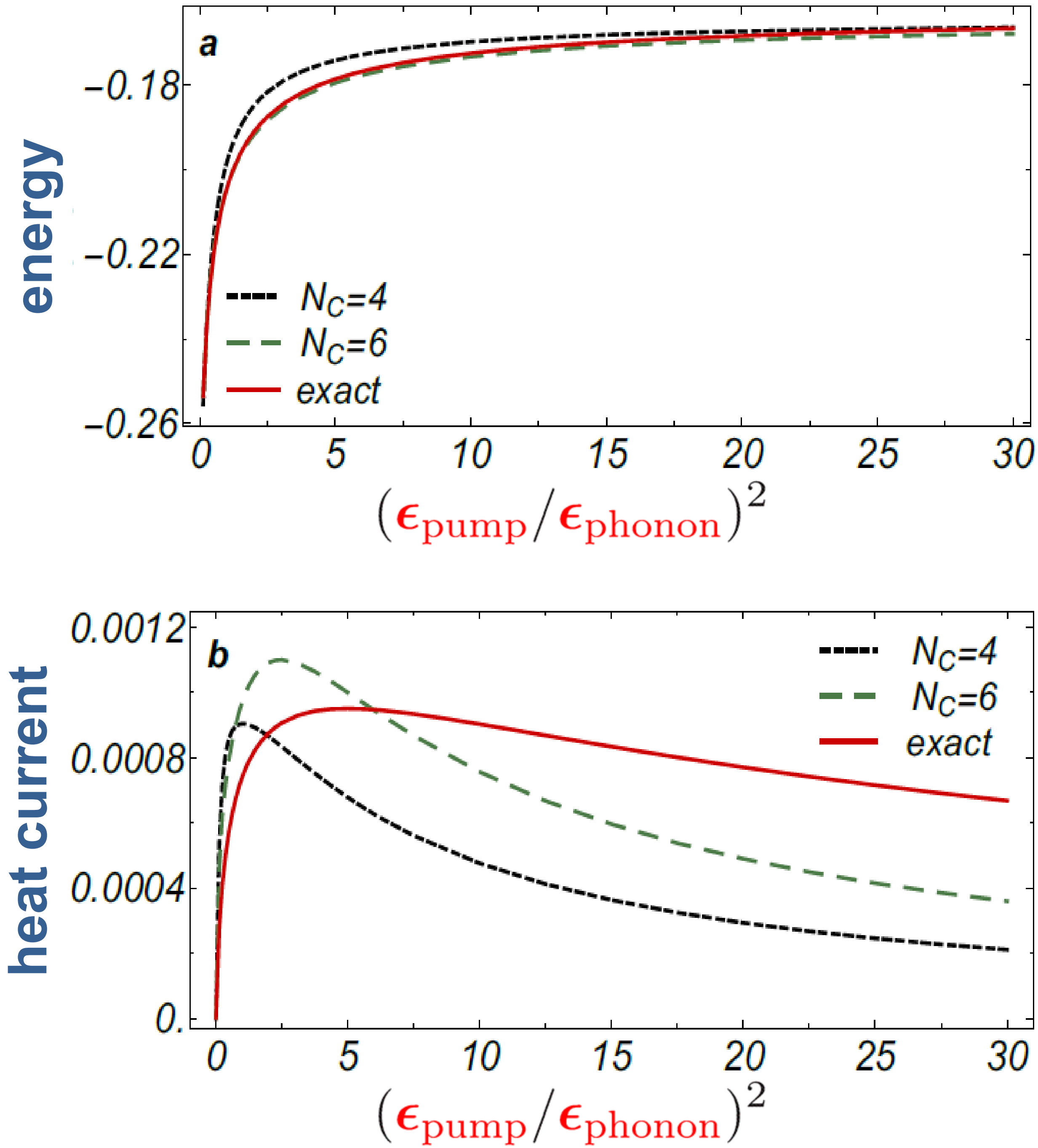


- heat current nominally of O(1) for $\epsilon_{\rm pump}, \epsilon_{\rm phonon} \to 0$
  $\epsilon_{\rm pump}/\epsilon_{\rm phonon} \sim 1$
- here: parameters not optimized
- needed: pumping ~ integrability breaking terms

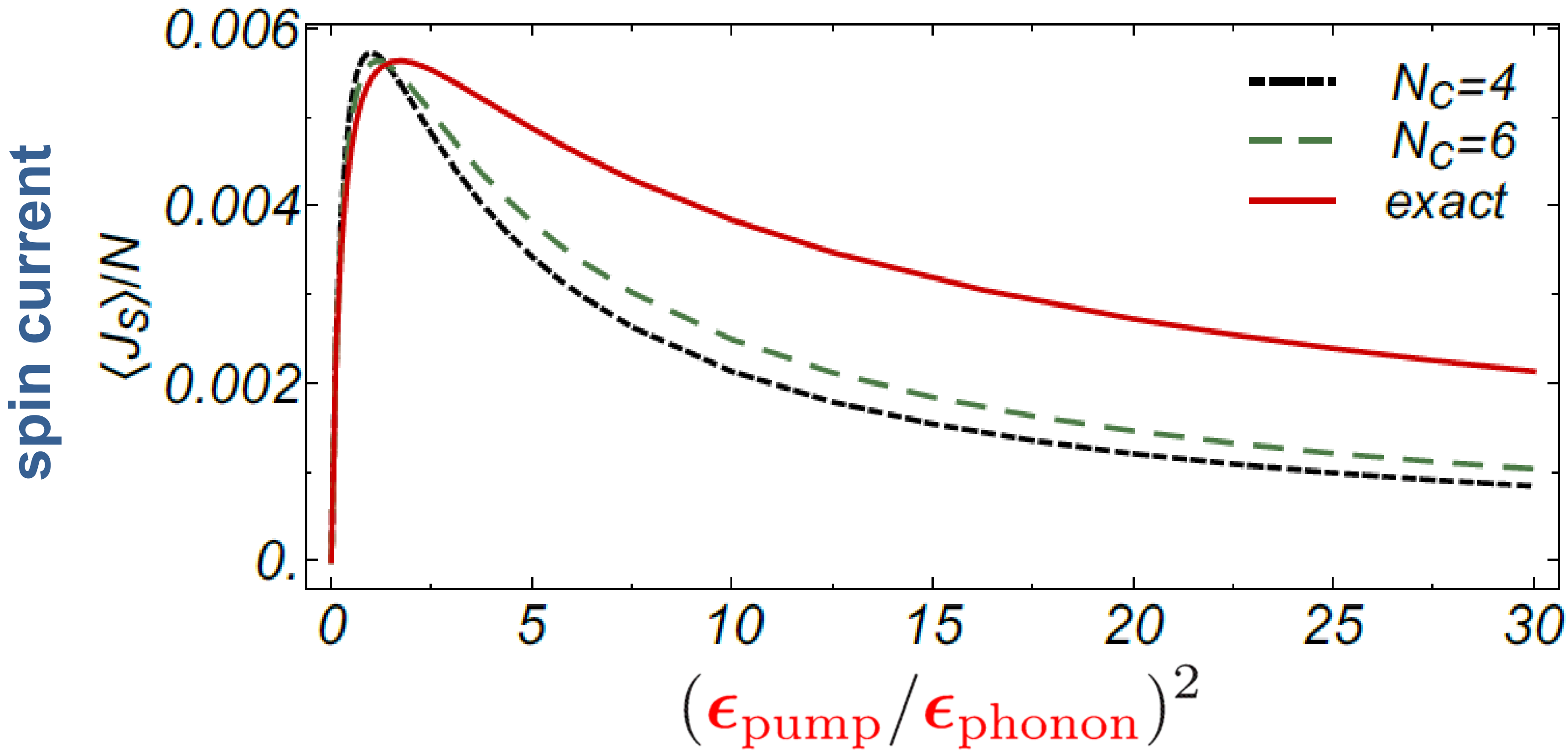


finite size effects: tiny for GGE

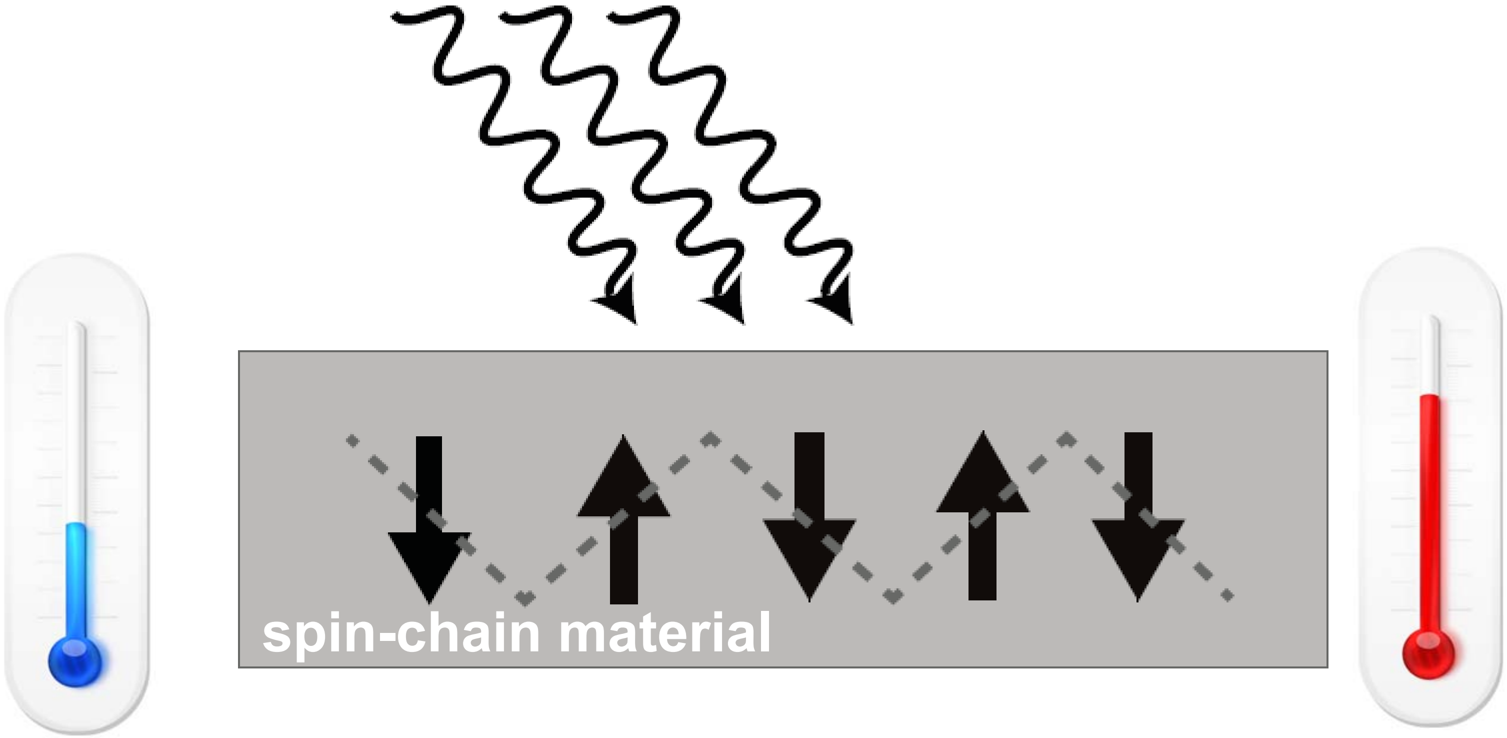
* this plot: without spin current contribution



- “exact“: use 7969 conservation laws of 12-site system (degenerate Liouvillian per-turbation theory)
- approximate: use GGE with Nc=4,6 conservation laws
- energy accurately described
- heat/spin current: qualitatively OK, but larger corrections



spin current for vanishing external field



control direction of temperature gradient by:
- external magnetic field
- polarization of incoming beam

use e.g. THz laser with $E \sim 10^8$ V/m

Numbers: heat currents

heat conductivity of cupper (300 K): $\kappa_{\mathrm{CU}} \approx 400 \frac{W}{mK}$

ultra-pure diamond from ^{12}C (300 K): $\kappa_{\mathrm{diamond}} \approx 3000 \frac{W}{mK}$

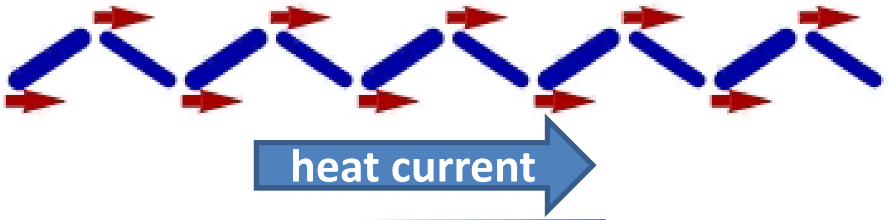
assume: $J \sim 20 \ldots 100\,\mathrm{K}, \quad J_H \sim 10^{-3} \ldots 10^{-2} \frac{J^2}{\hbar}$

distance of chains: $a = 5\,\mathrm{\AA}$

corresponding T-gradient in Cu:

$$\nabla T_{\mathrm{Cu}} = \frac{J_H}{a^2 \kappa_{\mathrm{CU}}} \sim 10^5 - 10^6 \frac{K}{m}$$

gigantic heat currents possible without T-gradients
if pumping ~ integrability breaking terms



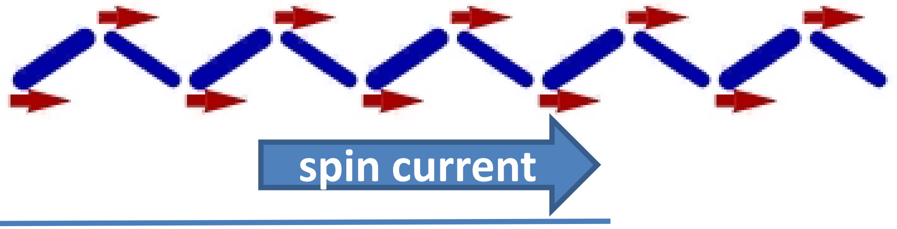
Numbers: spin currents

can, e.g., be created using spin-Hall effect in Pt

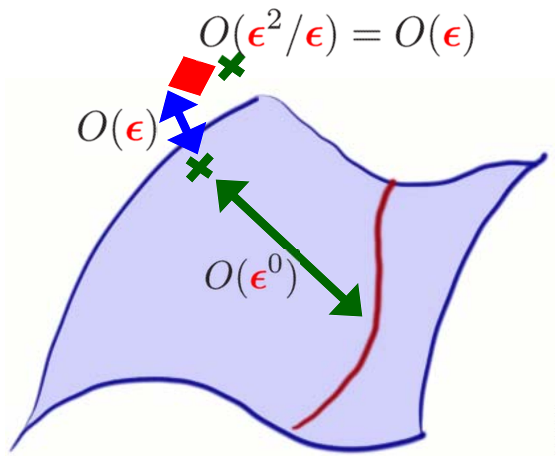
Hall angle $\alpha_s^{\mathrm{Pt}} \approx 10\,\%$ resistivity: $\rho^{\mathrm{Pt}} \approx 10\,\mu\Omega\,\mathrm{cm}$

Pt currents needed to create spin-currents of similar size:

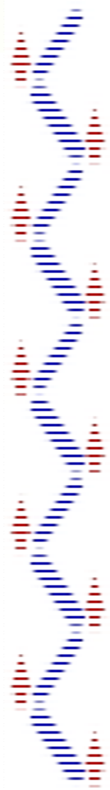
$$j^{\mathrm{Pt}} \sim 10^{11} A/m^2$$



conclusions



- perturbation theory for **weakly driven** systems
- many applications:
  - cavity QED
  - ultracold atoms (losses)
  - Floquet systems with weak (and strong) driving
  - excition, photon, magnon, … condensates
  - many pump-probe setups (two-temperature models)
- approximately integrable systems:
  activation of exotic conservation laws
- proposal for heat & spin pumps



outlook

- make integrability-based heat pump!
- theory of dynamics, inhomogeneous systems $\lambda_n(\vec{r}, t)$
- convergence issues, non-analytic corrections,…
- …

Lenarčič, Lange, A.R., arXiv:1706.05700
Lange, Lenarčič, A.R., Nature Comm. 8, 15767 (2017)